

FILE 'REGISTRY' ENTERED AT 11:47:36 ON 30 OCT 2006

L1	STRUCTURE UPLOADED
L2	0 S L1 FULL
L3	STRUCTURE UPLOADED
L4	0 S L3
L5	0 S L3 FULL
L6	STRUCTURE UPLOADED
L7	13 S L6
L8	STRUCTURE UPLOADED
L9	3 S L8 FULL
L10	STRUCTURE UPLOADED
L11	3 S L10 FULL
L12	STRUCTURE UPLOADED
L13	3 S L12 FULL

FILE 'MEDLINE, CAPLUS, EMBASE, BIOSIS, USPATFULL' ENTERED AT 12:01:11 ON 30 OCT 2006

FILE 'REGISTRY' ENTERED AT 12:01:19 ON 30 OCT 2006

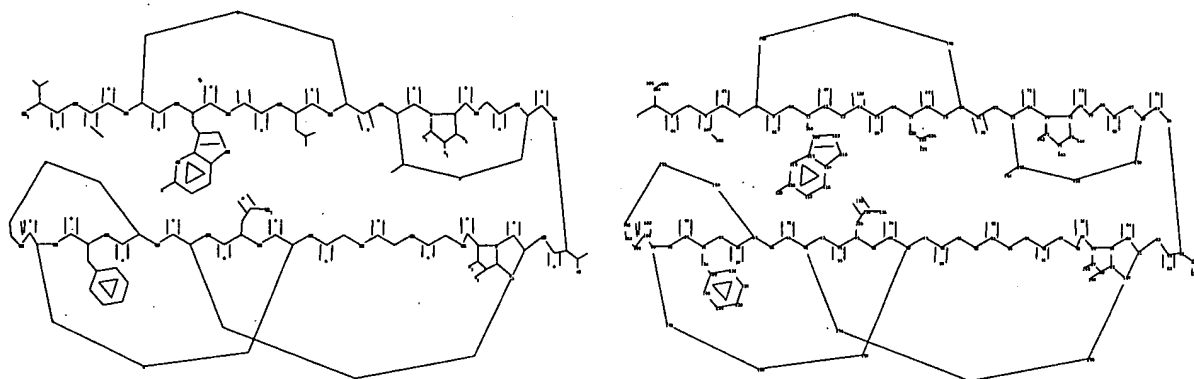
L14	3 S L11 OR L13
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FILE 'MEDLINE, CAPLUS, EMBASE, BIOSIS, USPATFULL' ENTERED AT 12:01:26 ON 30 OCT 2006

L15	7 S L14
L16	5 DUP REM L15 (2 DUPLICATES REMOVED)
L17	7 S ANTIBIOTIC 107891
L18	0 S L17 NOT L15

=>

Uploading C:\Program Files\Stnexp\Queries\11 035296\107891open.str



chain nodes :

1 2 3 4 5 6 7 21 22 29 30 31 32 33 62 63 64 65 66 67 68 69
70 71 79 80 81 82 83 84 90 91 92 93 94 95 96 97 98 103 104 105
106 107 108 110
120 121 122 123 124 125 129 130 131 132 134 142 143 144 145 146 147
154

ring nodes :

8 9 10 11 12 13 14 15 16 17 18 19 20 23 24 25 26 27 28 34 35
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56
57 58 59 60
61 72 73 74 75 76 77 78 85 86 87 88 89 99 100 101 102 109 111
112 113 114 115
116 117 118 119 126 127 128 133 135 136 137 138 139 140 141 150 151
152 153
155 156 157 158 159

chain bonds :

1-2 2-3 2-104 3-4 3-64 4-5 5-6 5-107 6-7 6-65 7-8 9-66 11-110 12-67
14-121 15-68 17-122 18-69 20-21 21-22 21-70 22-23 24-71 26-80 28-29
29-30 29-81 30-31
31-63 31-32 32-33 32-82 35-98 36-134 38-97 41-96 44-95 45-129 47-94
50-93 53-92 56-91
60-84 61-62 62-63 63-83 73-142 74-143 75-144 76-79 86-90 87-145 88-146
89-147 100-103
104-105 104-106 107-108 110-111 118-120 122-123 123-124 123-125 129-130
130-131 130-132
134-135 152-154

ring bonds :

8-9 8-150 9-10 10-11 11-12 12-13 13-14 14-15 15-16 16-17 17-18 18-19
19-20 20-151 23-24 23-152 24-25 25-72 25-73 26-27 26-78 27-28 28-153
34-35 34-99 35-36

36-37 37-38 38-39 39-40 39-159 40-41 41-42 42-43 42-156 43-44 44-45
 45-46 46-47 47-48
 48-49 48-157 49-50 50-51 51-52 52-53 53-54 54-55 55-56 56-57 57-58 58-86
 59-60 59-85
 59-89 60-61 61-155 72-75 72-76 73-74 74-75 76-77 77-78 85-86 85-87 87-88
 88-89 99-100
 99-158 100-101 101-102 102-141 109-150 109-151 111-112 111-115 112-113
 113-114 114-115
 114-116 115-119 116-117 117-118 118-119 126-152 126-153 127-155 127-156
 128-157 128-158
 133-141 133-159 135-136 135-140 136-137 137-138 138-139 139-140
 exact/norm bonds :
 1-2 3-4 3-64 4-5 6-7 6-65 7-8 8-9 8-150 9-10 9-66 10-11 11-12 12-13
 12-67 13-14 14-15 15-16 15-68 16-17 17-18 18-19 18-69 19-20 20-151 21-22
 21-70 22-23
 23-24 23-152 24-25 24-71 25-72 25-73 26-27 26-78 26-80 27-28 28-153
 29-30 29-81 30-31
 32-82 34-35 34-99 35-36 35-98 36-37 37-38 38-39 38-97 39-40 39-159 40-41
 41-42 41-96
 42-43 42-156 43-44 44-45 44-95 45-46 46-47 47-48 47-94 48-49 48-157
 49-50 50-51 50-93
 51-52 52-53 53-54 53-92 54-55 55-56 56-57 56-91 57-58 58-86 59-60 59-85
 59-89 60-61
 60-84 61-62 61-155 62-63 63-83 72-75 72-76 73-74 73-142 74-75 74-143
 75-144 76-77 76-79
 77-78 85-86 85-87 86-90 87-88 87-145 88-89 88-146 89-147 99-100 99-158
 100-101 100-103
 101-102 102-141 109-150 109-151 111-112 111-115 112-113 113-114 126-152
 126-153 127-155
 127-156 128-157 128-158 130-131 130-132 133-141 133-159
 exact bonds :
 2-3 2-104 5-6 5-107 11-110 14-121 17-122 20-21 28-29 31-63 31-32 32-33
 36-134 45-129 104-105 104-106 107-108 110-111 118-120 122-123 123-124
 123-125 129-130
 134-135 152-154
 normalized bonds :
 114-115 114-116 115-119 116-117 117-118 118-119 135-136 135-140 136-137
 137-138 138-139 139-140

G1:H,OH

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
 10:Atom
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
 20:Atom 21:CLASS
 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
 31:CLASS
 32:CLASS 33:CLASS 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom
 41:Atom 42:Atom
 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom
 52:Atom 53:Atom
 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:CLASS
 63:CLASS 64:CLASS
 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:Atom
 73:Atom 74:Atom
 75:Atom 76:Atom 77:Atom 78:Atom 79:CLASS 80:CLASS 81:CLASS 82:CLASS
 83:CLASS 84:CLASS
 85:Atom 86:Atom 87:Atom 88:Atom 89:Atom 90:CLASS 91:CLASS 92:CLASS 93:CLASS
 94:CLASS 95:CLASS
 96:CLASS 97:CLASS 98:CLASS 99:Atom 100:Atom 101:Atom 102:Atom 103:CLASS
 104:CLASS
 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:Atom 110:CLASS 111:Atom 112:Atom
 113:Atom 114:Atom

115:Atom 116:Atom 117:Atom 118:Atom 119:Atom 120:CLASS 121:CLASS 122:CLASS
123:CLASS
124:CLASS 125:CLASS 126:Atom 127:Atom 128:Atom 129:CLASS 130:CLASS 131:CLASS
132:CLASS 133:Atom
134:CLASS 135:Atom 136:Atom 137:Atom 138:Atom 139:Atom 140:Atom 141:Atom
142:CLASS
143:CLASS 144:CLASS 145:CLASS 146:CLASS 147:CLASS 150:Atom 151:Atom 152:Atom
153:Atom 154:CLASS
155:Atom 156:Atom 157:Atom 158:Atom 159:Atom